

## Questionnaire for Evaluation of Quality Criteria for Mass Spectra in EUROCarbDB

Name.....

Institution.....Position.....

### A. Criteria scientists use to evaluate the quality of an acquired mass spectrum

1. Which of the following parameters do you take into account for evaluating the quality of a spectrum?

Parameter		
(a) Whether the general appearance of the spectrum meet my expectation	<input type="checkbox"/> yes	<input type="checkbox"/> no
(b) Signal to noise ratio of the whole spectrum	<input type="checkbox"/> yes	<input type="checkbox"/> no
(c) Signal to noise ratio of the expected peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(d) Mass calibration of the spectrum	<input type="checkbox"/> yes	<input type="checkbox"/> no
(e) Shape of peaks (i.e. tailing)	<input type="checkbox"/> yes	<input type="checkbox"/> no
(d) Resolution of the peaks in the whole spectrum	<input type="checkbox"/> yes	<input type="checkbox"/> no
(e) Resolution of the expected peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(f) Occurrence of known impurities	<input type="checkbox"/> yes	<input type="checkbox"/> no
(g) Correct isotopic patterns for expected peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(h) Reproducibility of the Acquisition	<input type="checkbox"/> yes	<input type="checkbox"/> no
Please list if others:		
(i)	<input type="checkbox"/> yes	<input type="checkbox"/> no
(j)	<input type="checkbox"/> yes	<input type="checkbox"/> no
(k)	<input type="checkbox"/> yes	<input type="checkbox"/> no

2. Rank the top 5 parameters you always take into account (Please specify for different techniques, if parameters differ)

	tech: _____	tech: _____	tech: _____
1.	_____	_____	_____
2.	_____	_____	_____
3.	_____	_____	_____
4.	_____	_____	_____
5.	_____	_____	_____

### B. Criteria glycoscientists use to evaluate the quality of the annotation of a mass spectrum

3. Which of the following parameters do you take into account to evaluate the quality of the annotation of a spectrum?

Parameter		
(a) Whether the annotation meet my expectation	<input type="checkbox"/> yes	<input type="checkbox"/> no
(b) Number of annotated peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(c) Percentage of annotated peaks with good signal to noise ratio	<input type="checkbox"/> yes	<input type="checkbox"/> no
(d) Mass accuracy of annotated peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(e) All the expected peaks are found in the spectra	<input type="checkbox"/> yes	<input type="checkbox"/> no
(f) All the relevant peaks are assigned	<input type="checkbox"/> yes	<input type="checkbox"/> no
Please list if others:		
(g)	<input type="checkbox"/> yes	<input type="checkbox"/> no
(h)	<input type="checkbox"/> yes	<input type="checkbox"/> no
(i)	<input type="checkbox"/> yes	<input type="checkbox"/> no

4. Rank the top 3 parameters you always take into account

1. \_\_\_\_\_
2. \_\_\_\_\_
3. \_\_\_\_\_

### C. Criteria glycoscientists would focus on when retrieving data from EUROCarbDB

5. Which of the following parameters that can be derived automatically would you like to view when you retrieve an annotated spectrum from a database?

Parameter		
(a) Signal to noise ratio of the whole spectrum and for different regions of the spectrum	<input type="checkbox"/> yes	<input type="checkbox"/> no
(b) Statistics for resolution and shape of peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(c) Percentage of annotated peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(d) Accuracy of mass for annotated signals	<input type="checkbox"/> yes	<input type="checkbox"/> no
(e) Analysis of isotopic patterns for annotated peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(d) Sequence coverage	<input type="checkbox"/> yes	<input type="checkbox"/> no
(e) Statistics of missing peaks	<input type="checkbox"/> yes	<input type="checkbox"/> no
(f) Relative abundance of multiply charge states for detected ions	<input type="checkbox"/> yes	<input type="checkbox"/> no
Please list if others:		
(g)	<input type="checkbox"/> yes	<input type="checkbox"/> no
(h)	<input type="checkbox"/> yes	<input type="checkbox"/> no
(i)	<input type="checkbox"/> yes	<input type="checkbox"/> no

6. a) Is it necessary / helpful to assign a general quality score value to a spectrum?

- Yes, a general score value is helpful
- No, I won't use such a value
- A general quality score value is imprecise, the score values should be categorized.

I propose the following categories:

_____	_____
_____	_____
_____	_____

b) Should the quality score value(s) be calculated separately for different experimental techniques?

- yes /  no

7. Comments

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Thank you for contributing to our initiative to evaluate quality criteria for mass spectra used by glycoscientists. The results of this survey will be presented on the project homepage [www.eurocarbodb.org](http://www.eurocarbodb.org)

The EUROCarbDB - Team